```
Connecting via Winsock to STN


Welcome to STN International!  Enter x:x

LOGINID:ssspta1617srh

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2


* * * * * * * * * *   Welcome to STN International   * * * * * * * * * *

 NEWS  1           Web Page URLs for STN Seminar Schedule - N. America
 NEWS  2           "Ask CAS" for self-help around the clock
 NEWS  3  JAN 27   Source of Registration (SR) information in REGISTRY updated
                   and searchable
 NEWS  4  JAN 27   A new search aid, the Company Name Thesaurus, available in
                   CA/CAplus
 NEWS  5  FEB 05   German (DE) application and patent publication number format
                   changes
 NEWS  6  MAR 03   MEDLINE and LMEDLINE reloaded
 NEWS  7  MAR 03   MEDLINE file segment of TOXCENTER reloaded
 NEWS  8  MAR 03   FRANCEPAT now available on STN
 NEWS  9  MAR 29   Pharmaceutical Substances (PS) now available on STN
 NEWS 10  MAR 29   WPIFV now available on STN
 NEWS 11  MAR 29   New monthly current-awareness alert (SDI) frequency in RAPRA
 NEWS 12  APR 26   PROMT: New display field available
 NEWS 13  APR 26   IFIPAT/IFIUDB/IFICDB: New super search and display field
                   available
 NEWS 14  APR 26   LITALERT now available on STN
 NEWS 15  APR 27   NLDB: New search and display fields available
 NEWS 16  May 10   PROUSDDR now available on STN
 NEWS 17  May 19   PROUSDDR: One FREE connect hour, per account, in both May
                   and June 2004
 NEWS 18  May 12   EXTEND option available in structure searching
 NEWS 19  May 12   Polymer links for the POLYLINK command completed in REGISTRY
 NEWS 20  May 17   FRFULL now available on STN

 NEWS EXPRESS  MARCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT
               MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
               AND CURRENT DISCOVER FILE IS DATED 26 APRIL 2004
 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS INTER    General Internet Information
 NEWS LOGIN    Welcome Banner and News Items
 NEWS PHONE    Direct Dial and Telecommunication Network Access to STN
 NEWS WWW      CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that
specific topic.

  All use of STN is subject to the provisions of the STN Customer
  agreement.  Please note that this agreement limits use to scientific
  research.  Use for software development or design or implementation
  of commercial gateways or other similar uses is prohibited and may
  result in loss of user privileges and other penalties.

  * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 15:01:15 ON 25 MAY 2004
```

```
=> fil reg
COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                           ENTRY    SESSION
FULL ESTIMATED COST                                         0.21       0.21

FILE 'REGISTRY' ENTERED AT 15:01:47 ON 25 MAY 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   24 MAY 2004  HIGHEST RN 685504-43-2
DICTIONARY FILE UPDATES:  24 MAY 2004  HIGHEST RN 685504-43-2

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

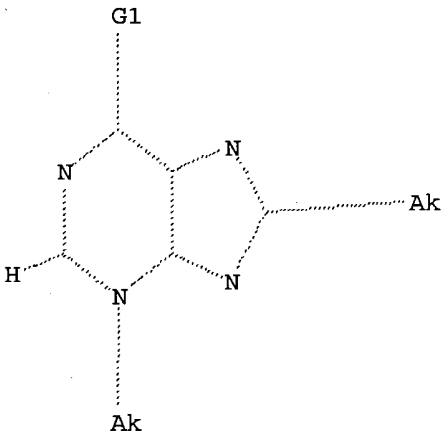
Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\hypoxanthine.str

L1      STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1               STR
```




```
G1 O,S


Structure attributes must be viewed using STN Express query preparation.


=> s l1
SAMPLE SEARCH INITIATED 15:02:42 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -    5489 TO ITERATE

 18.2% PROCESSED    1000 ITERATIONS                                0 ANSWERS
```

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 105339 TO 114221
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

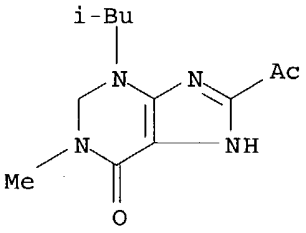
=> s l1 full
FULL SEARCH INITIATED 15:02:46 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 111306 TO ITERATE

100.0% PROCESSED 111306 ITERATIONS 39 ANSWERS
SEARCH TIME: 00.00.05

L3 39 SEA SSS FUL L1

=> d scan

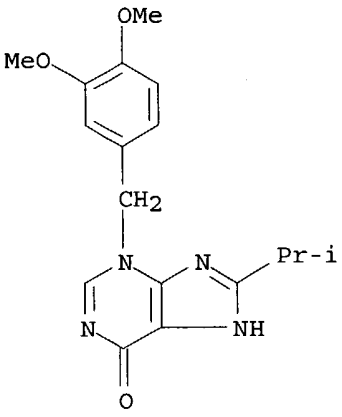
L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 6H-Purin-6-one, 8-acetyl-1,2,3,7-tetrahydro-1-methyl-3-(2-methylpropyl)-(9CI)
MF C12 H18 N4 O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

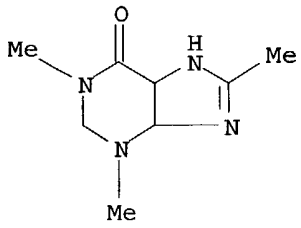
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):38

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 6H-Purin-6-one, 3-[(3,4-dimethoxyphenyl)methyl]-3,7-dihydro-8-(1-methylethyl)- (9CI)
MF C17 H20 N4 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

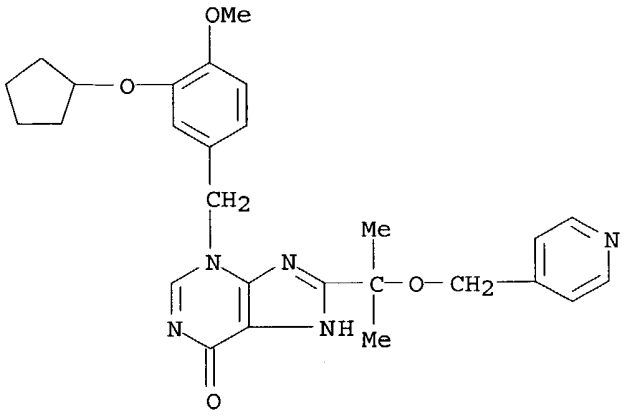
L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 1H-Purinium, 4,5,6,7-tetrahydro-1,3,8-trimethyl-6-oxo-, iodide (9CI)
MF C8 H13 N4 O . I



● I^-

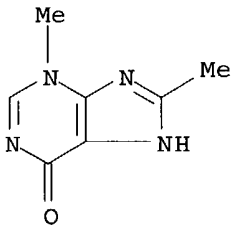
*** FRAGMENT DIAGRAM IS INCOMPLETE ***

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 6H-Purin-6-one, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-3,7-dihydro-8-[1-methyl-1-(4-pyridinylmethoxy)ethyl]- (9CI)
MF C27 H31 N5 O4



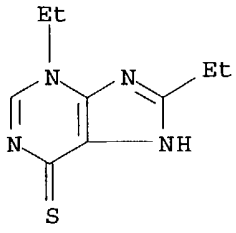
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 6H-Purin-6-one, 3,7-dihydro-3,8-dimethyl- (9CI)
MF C7 H8 N4 O



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

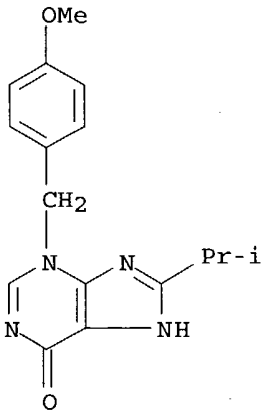
L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 6H-Purine-6-thione, 3,8-diethyl-3,7-dihydro- (9CI)
MF C9 H12 N4 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

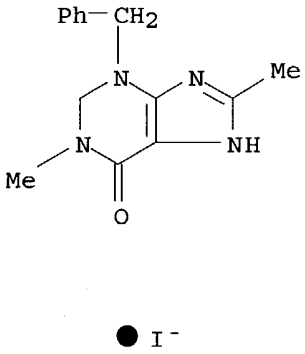
L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 6H-Purin-6-one, 3,7-dihydro-3-[(4-methoxyphenyl)methyl]-8-(1-methylethyl)-
(9CI)

MF C16 H18 N4 O2



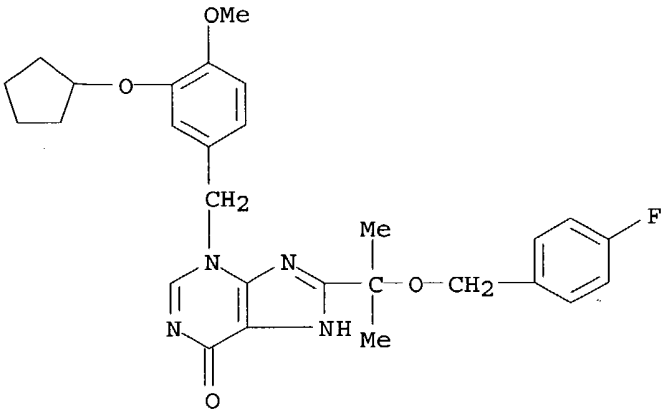
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 1H-Purinium, 6,7-dihydro-1,8-dimethyl-6-oxo-3-(phenylmethyl)-, iodide (9CI)
MF C14 H15 N4 O . I



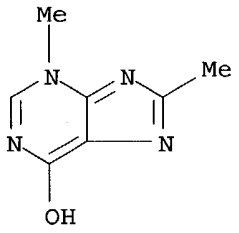
*** FRAGMENT DIAGRAM IS INCOMPLETE ***

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 6H-Purin-6-one, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-8-[1-[(4-fluorophenyl)methoxy]-1-methylethyl]-3,7-dihydro- (9CI)
MF C28 H31 F N4 O4



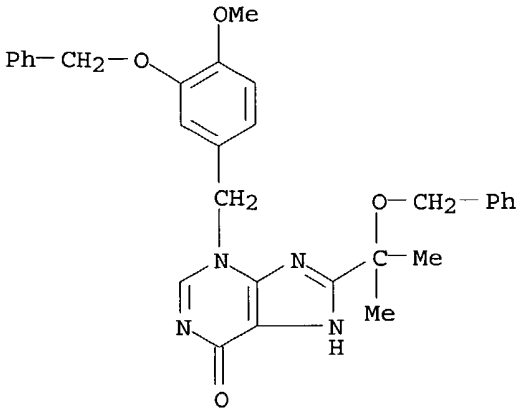
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 3H-Purin-6-ol, 3,8-dimethyl- (9CI)
MF C7 H8 N4 O



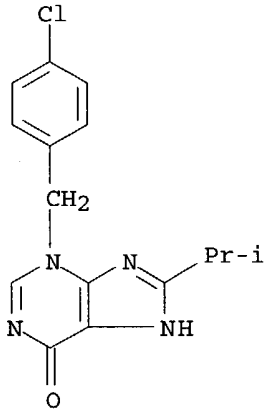
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 6H-Purin-6-one, 3,7-dihydro-3-[[4-methoxy-3-(phenylmethoxy)phenyl]methyl]-8-[1-methyl-1-(phenylmethoxy)ethyl]- (9CI)
MF C30 H30 N4 O4



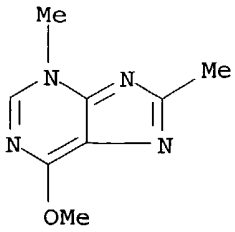
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 6H-Purin-6-one, 3-[(4-chlorophenyl)methyl]-3,7-dihydro-8-(1-methylethyl)-(9CI)
MF C15 H15 Cl N4 O



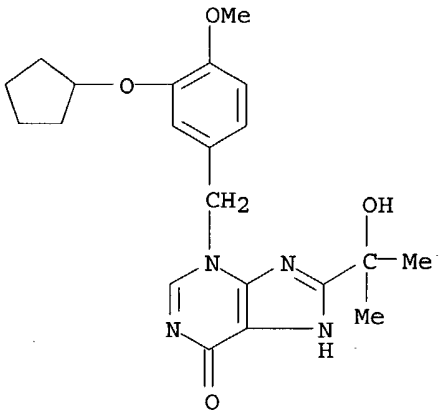
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 3H-Purine, 6-methoxy-3,8-dimethyl- (9CI)
MF C8 H10 N4 O



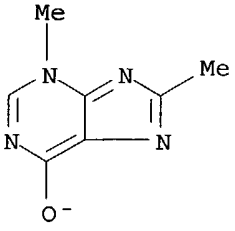
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 6H-Purin-6-one, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-3,7-dihydro-8-(1-hydroxy-1-methylethyl)- (9CI)
MF C21 H26 N4 O4



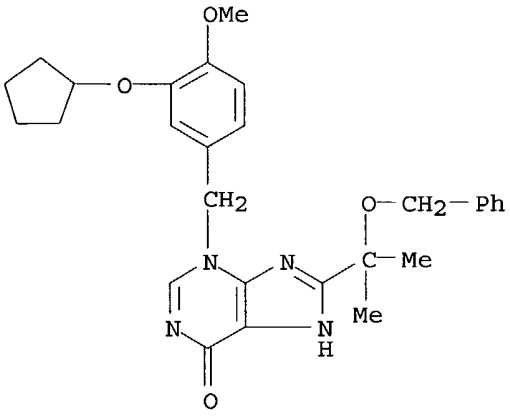
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 3H-Purin-6-ol, 3,8-dimethyl-, ion(1-) (9CI)
MF C7 H7 N4 O



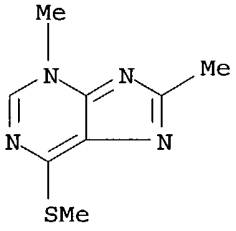
L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 6H-Purin-6-one, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-3,7-dihydro-8-[1-methyl-1-(phenylmethoxy)ethyl]- (9CI)

MF C28 H32 N4 O4



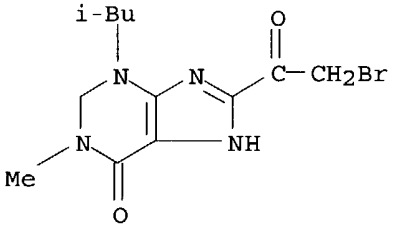
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 3H-Purine, 3,8-dimethyl-6-(methylthio)- (7CI, 8CI, 9CI)
MF C8 H10 N4 S



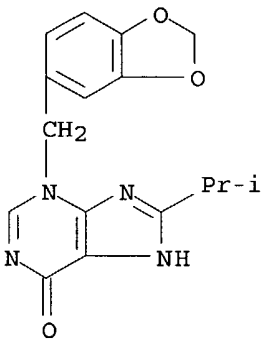
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 6H-Purin-6-one, 8-(bromoacetyl)-1,2,3,7-tetrahydro-1-methyl-3-(2-methylpropyl)- (9CI)
MF C12 H17 Br N4 O2



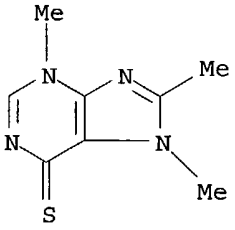
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 6H-Purin-6-one, 3-(1,3-benzodioxol-5-ylmethyl)-3,7-dihydro-8-(1-methylethyl)- (9CI)
MF C16 H16 N4 O3



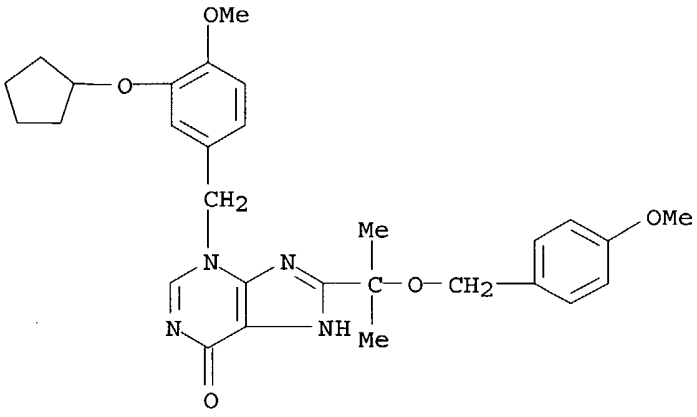
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 6H-Purine-6-thione, 3,7-dihydro-3,7,8-trimethyl- (9CI)
MF C8 H10 N4 S
CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

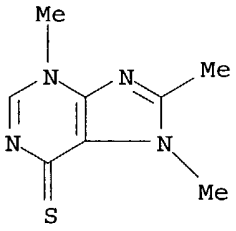
L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 6H-Purin-6-one, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-3,7-dihydro-8-[1-[(4-methoxyphenyl)methoxy]-1-methylethyl]- (9CI)
MF C29 H34 N4 O5



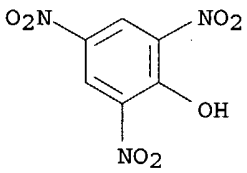
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Purine-6(3H)-thione, 3,7,8-trimethyl-, picrate (7CI, 8CI)
MF C8 H10 N4 S . C6 H3 N3 O7

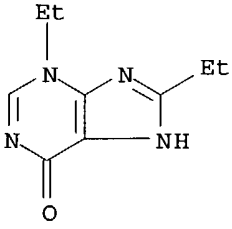
CM 1



CM 2

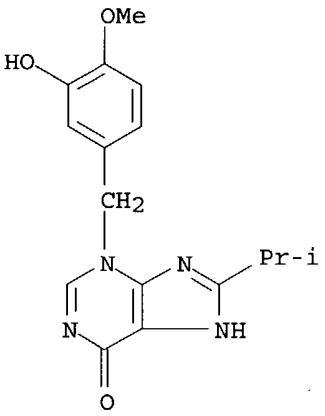


L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 6H-Purin-6-one, 3,8-diethyl-3,7-dihydro- (9CI)
MF C9 H12 N4 O



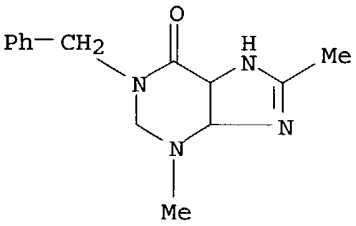
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 6H-Purin-6-one, 3,7-dihydro-3-[(3-hydroxy-4-methoxyphenyl)methyl]-8-(1-methylethyl)- (9CI)
MF C16 H18 N4 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

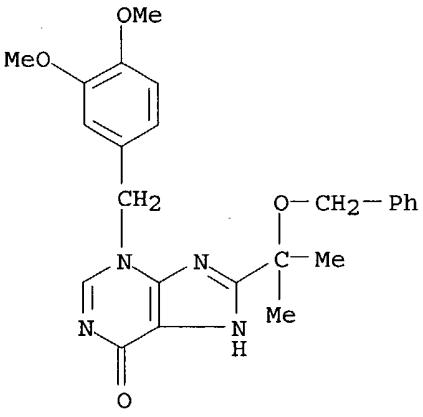
L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 1H-Purinium, 4,5,6,7-tetrahydro-3,8-dimethyl-6-oxo-1-(phenylmethyl)-, bromide (9CI)
MF C14 H17 N4 O . Br



● Br^-

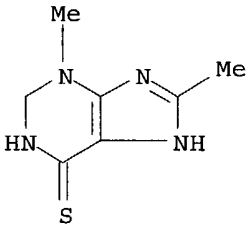
*** FRAGMENT DIAGRAM IS INCOMPLETE ***

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 6H-Purin-6-one, 3-[(3,4-dimethoxyphenyl)methyl]-3,7-dihydro-8-[1-methyl-1-(phenylmethoxy)ethyl]- (9CI)
MF C24 H26 N4 O4



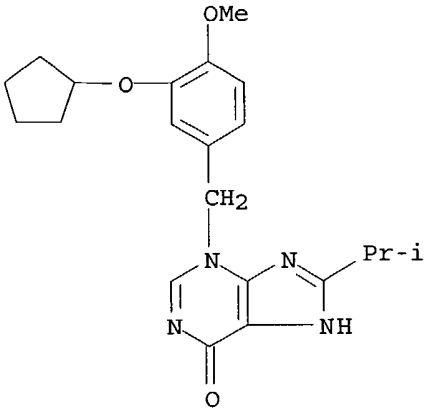
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 6H-Purine-6-thione, 1,2,3,7-tetrahydro-3,8-dimethyl- (9CI)
MF C7 H10 N4 S



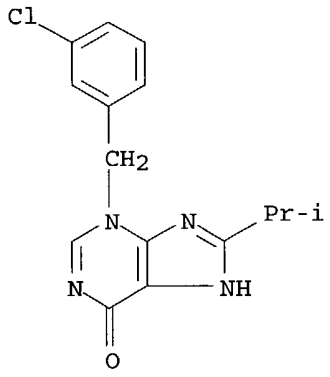
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 6H-Purin-6-one, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-3,7-dihydro-8-(1-methylethyl)- (9CI)
MF C21 H26 N4 O3



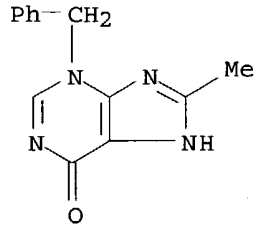
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 6H-Purin-6-one, 3-[(3-chlorophenyl)methyl]-3,7-dihydro-8-(1-methylethyl)-
(9CI)
MF C15 H15 Cl N4 O



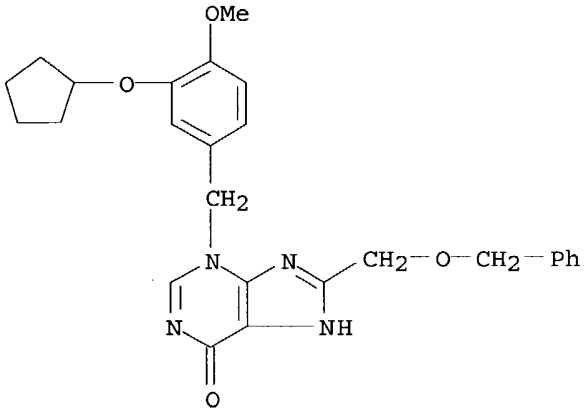
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 6H-Purin-6-one, 3,7-dihydro-8-methyl-3-(phenylmethyl)- (9CI)
MF C13 H12 N4 O



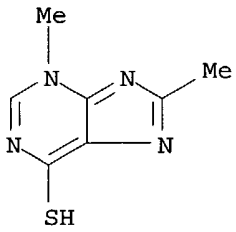
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 6H-Purin-6-one, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-3,7-dihydro-8-[(phenylmethoxy)methyl]- (9CI)
MF C26 H28 N4 O4



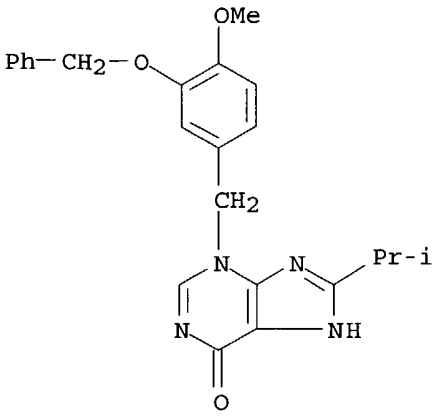
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 3H-Purine-6-thiol, 3,8-dimethyl- (9CI)
MF C7 H8 N4 S



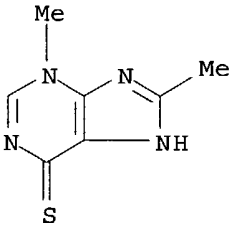
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 6H-Purin-6-one, 3,7-dihydro-3-[[4-methoxy-3-(phenylmethoxy)phenyl]methyl]-8-(1-methylethyl)- (9CI)
MF C23 H24 N4 O3



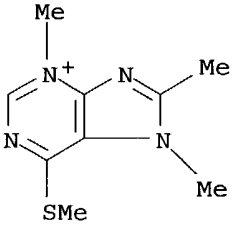
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 6H-Purine-6-thione, 1,3-dihydro-3,8-dimethyl- (9CI)
MF C7 H8 N4 S



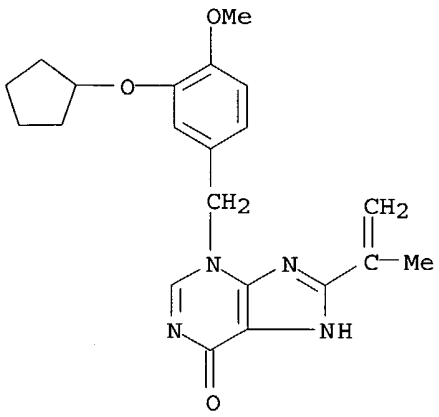
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 3,7,8-Trimethyl-6-(methylthio)purinium iodide (7CI)
MF C9 H13 N4 S . I



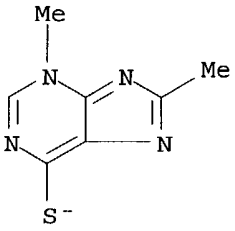
● I^-

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 6H-Purin-6-one, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-3,7-dihydro-8-(1-methylethenyl)- (9CI)
MF C21 H24 N4 O3

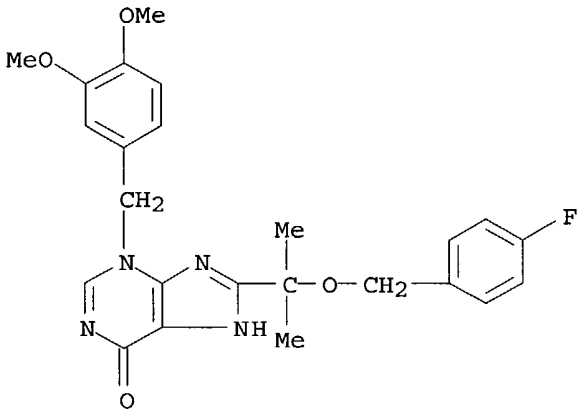


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 3H-Purine-6-thiol, 3,8-dimethyl-, ion(1-) (9CI)
MF C7 H7 N4 S

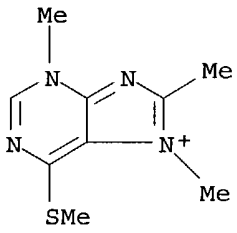


L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 6H-Purin-6-one, 3-[(3,4-dimethoxyphenyl)methyl]-8-[1-[(4-fluorophenyl)methoxy]-1-methylethyl]-3,7-dihydro- (9CI)
MF C24 H25 F N4 O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 39 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Purinium, 3,7,8-trimethyl-6-(methylthio)-, iodide (8CI)
MF C9 H13 N4 S . I



ALL ANSWERS HAVE BEEN SCANNED

=> fil medlin hcapl uspatf wpids

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	156.26	156.47

FILE 'MEDLINE' ENTERED AT 15:03:50 ON 25 MAY 2004

FILE 'HCAPLUS' ENTERED AT 15:03:50 ON 25 MAY 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE 'USPATFULL' ENTERED AT 15:03:50 ON 25 MAY 2004

FILE 'WPIDS' ENTERED AT 15:03:50 ON 25 MAY 2004

```
=> s l3
SAMPLE SEARCH INITIATED 15:03:56 FILE 'WPIDS'
SAMPLE SCREEN SEARCH COMPLETED -    311 TO ITERATE

100.0% PROCESSED     311 ITERATIONS                              3 ANSWERS
SEARCH TIME: 00.00.07

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         2583 TO     3637
PROJECTED ANSWERS:               3 TO       81

L4          47 L3

=> dup rem l4
PROCESSING COMPLETED FOR L4
L5           46 DUP REM L4 (1 DUPLICATE REMOVED)

=> s l5 not py>1999
L6          22 L5 NOT PY>1999

=> d ibib abs hitstr 15-22

L6   ANSWER 15 OF 22  USPATFULL on STN
ACCESSION NUMBER:       1999:96373  USPATFULL
TITLE:                  Chemical compounds having PDE-IV inhibition activity
INVENTOR(S):            Cavalla, David, Cambridge, United Kingdom
                        Gehrig, Anddre, Basel, Switzerland
                        Chasin, Mark, Manalapan, NJ, United States
                        Hofer, Peter, Liestal, Switzerland
                        Wintergest, Peter, Basel, Switzerland
PATENT ASSIGNEE(S):     Euro-Celtique, S.A., Luxembourg, Luxembourg (non-U.S.
                        corporation)

                             NUMBER        KIND    DATE
                        ---------------- ------ --------
PATENT INFORMATION:     US 5939422                19990817
                        WO 9500516                19950105
APPLICATION INFO.:      US 1996-578580            19960408  (8)
                        WO 1994-GB1334            19940621
                                                  19960408  PCT 371 date
                                                  19960408  PCT 102(e) date

                               NUMBER         DATE
                        ------------------ --------
PRIORITY INFORMATION:   GB 1993-12853      19930622
DOCUMENT TYPE:          Utility
FILE SEGMENT:           Granted
PRIMARY EXAMINER:       Berch, Mark L
LEGAL REPRESENTATIVE:   Davidson, Davidson & Kappel, LLC
NUMBER OF CLAIMS:       50
EXEMPLARY CLAIM:        1,3
NUMBER OF DRAWINGS:     2 Drawing Figure(s); 2 Drawing Page(s)
LINE COUNT:             1819
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB     Disclosed is a compound of the formula (I): wherein

       R.sub.3, R.sub.6a and R.sub.8 are the same or different and represent a
       C.sub.2-8 alkyl which is unbranched or branched and unsubstituted or
       substituted; C.sub.3-8 cycloalkyl which is unsubstituted or substituted;
       C.sub.4-8 cycloalkylalkyl wherein the cycloalkyl portion is
       unsubstituted or substituted; aryl which is unsubstituted or
       substituted; aralkyl C.sub.1-4 ; heterocyclyl; and heterocyclylalkyl
```

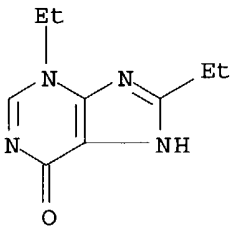
(C.sub.1 -C.sub.4)

R.sub.6b represents H or R.sub.6a, or together R.sub.6b, N, and R.sub.6a make a C.sub.3 -C.sub.8 ring containing from one to three nitrogen atoms, from zero to two oxygen atoms, from zero to two sulfur atoms, which is optionally substituted;

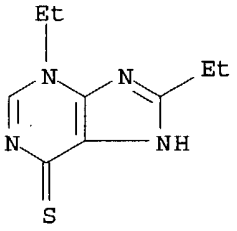
and where aryl is phenyl or naphthyl, the heterocyclyl is a 5, 6 or 7 membered ring including from one to three nitrogen atoms, and from zero to two oxygen atoms, from zero to two sulfur atoms, and can be substituted as in aryl on the carbons or nitrogens of that ring;

or a pharmaceutically acceptable salt thereof.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **162279-42-7P 162279-43-8P**
(preparation of purines, isoguanines, and dithioxanthines as phosphodiesterase-IV inhibitors)
RN 162279-42-7 USPATFULL
CN 6H-Purin-6-one, 3,8-diethyl-3,7-dihydro- (9CI) (CA INDEX NAME)



RN 162279-43-8 USPATFULL
CN 6H-Purine-6-thione, 3,8-diethyl-3,7-dihydro- (9CI) (CA INDEX NAME)



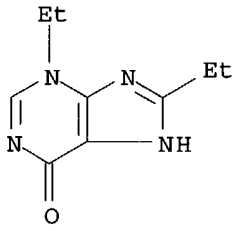
L6 ANSWER 16 OF 22 USPATFULL on STN
ACCESSION NUMBER: 1999:78756 USPATFULL
TITLE: Aryl pyrazole compound for inhibiting phosphodiesterase IV and methods of using same
INVENTOR(S): Cavalla, David John, Cambridge, United Kingdom
Chasin, Mark, Manalapan, NJ, United States
Dolby, Lloyd J., Eugene, OR, United States
Frith, Richard William, Cambridge, United Kingdom
PATENT ASSIGNEE(S): Euro-Celtique, S.A., Luxembourg, Luxembourg (non-U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 5922751		19990713
APPLICATION INFO.:	US 1997-782502		19970110 (8)

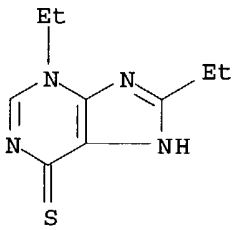
RELATED APPLN. INFO.: Continuation of Ser. No. US 1995-486184, filed on 7 Jun 1995, now abandoned which is a continuation-in-part of

Ser. No. US 1994-265641, filed on 24 Jun 1994, now abandoned
DOCUMENT TYPE: Utility
FILE SEGMENT: Granted
PRIMARY EXAMINER: Dees, Jose' G.
ASSISTANT EXAMINER: Stockton, Laura L.
LEGAL REPRESENTATIVE: Davidson, Davidson & Kappel, LLC
NUMBER OF CLAIMS: 24
EXEMPLARY CLAIM: 1
LINE COUNT: 1595
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB Novel compounds which are effective PDE IV inhibitors are disclosed The compounds possess similar or improved PDE IV inhibition as compared to rolipram, with improved selectivity with regard to, e.g., PDE III inhibition. Preferred compounds are 3-(3-cyclopentyloxy-4-methoxy-benzylamino)-4-hydroxymethyl pyrazole and 3-(3-cyclopentyloxy-4-methoxybenzylamino)-4-methoxymethylpyrazole.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **162279-42-7P 162279-43-8P**
(preparation of purines, isoguanines, and dithioxanthines as phosphodiesterase-IV inhibitors)
RN 162279-42-7 USPATFULL
CN 6H-Purin-6-one, 3,8-diethyl-3,7-dihydro- (9CI) (CA INDEX NAME)



RN 162279-43-8 USPATFULL
CN 6H-Purine-6-thione, 3,8-diethyl-3,7-dihydro- (9CI) (CA INDEX NAME)



L6 ANSWER 17 OF 22 USPATFULL on STN
ACCESSION NUMBER: 1999:40431 USPATFULL
TITLE: Heterocyclic compounds for inhibiting phosphodiesterase IV
INVENTOR(S): Cavalla, David John, Cambridge, England
Dolby, Lloyd J., Eugene, OR, United States
Chasin, Mark, Manalapan, NJ, United States
PATENT ASSIGNEE(S): Euro-Celtique, S.A., Luxembourg, Luxembourg (non-U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 5889014		19990330

APPLICATION INFO.: US 1996-716902 19960920 (8)
RELATED APPLN. INFO.: Division of Ser. No. US 1995-370952, filed on 10 Jan 1995, now patented, Pat. No. US 5591776 which is a continuation-in-part of Ser. No. US 1994-321730, filed on 12 Oct 1994, now patented, Pat. No. US 5665737
DOCUMENT TYPE: Utility
FILE SEGMENT: Granted
PRIMARY EXAMINER: Gupta, Yogendra N.
LEGAL REPRESENTATIVE: Davidson, Davidson & Kappel, LLC
NUMBER OF CLAIMS: 16
EXEMPLARY CLAIM: 1
LINE COUNT: 914
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Novel compounds which are effective PDE IV inhibitors are disclosed. The compounds have the formula: ##STR1## wherein: R.sub.1 and R.sub.2 may be the same or different and each is selected from the group consisting of hydrogen, saturated or unsaturated straight-chain or branched C.sub.1-12 alkyl groups, cycloalkyl and cycloalkyl-alkyl groups containing from 3 to 10 carbon atoms in the cycloalkyl moiety;

R.sub.3 is hydrogen, halogen, or a saturated or unsaturated straight-chain or branched C.sub.1-12 alkyl group, a cycloalkyl and cycloalkyl-alkyl groups containing from 3 to 7 carbon atoms in the cycloalkyl moiety;

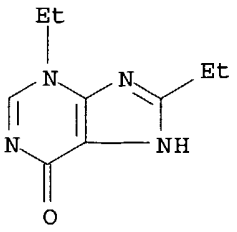
R.sub.4 is a phenyl or benzyl or a 6-membered heteroaryl which may be unsubstituted or substituted with one or more halogen atoms, alkyl groups, nitro groups, hydroxyl groups, cyano groups, carboxyl groups, alkoxy group, alkoxycarbonyl, amido, carboxamido, substituted or unsubstituted amino groups, cycloalkyl and cycloalkyl-alkyl groups containing from 3 to 10 carbon atoms in the cycloalkyl moiety, aryl or aralkyl groups preferably containing from about 6 to about 10 carbon atoms, or heterocyclic groups containing nitrogen, oxygen or sulfur in the ring; said alkyl, cycloalkyl, cycloalkyl-alkyl, aryl, and arylalkyl groups being unsubstituted or substituted by halogen atoms, hydroxyl groups, cyano groups, carboxyl groups, alkoxy groups, alkoxycarbonyl, carboxamido or substituted or unsubstituted amino groups, or one or more lower alkyl groups having from 1 to 3 carbon atoms;

Z is selected from the group consisting of --CH.sub.2 CO--, --NHCH.sub.2 --, --CH.sub.2 NH--, --CH.sub.2 CONH--, --CH.sub.2 NHCO--, --CH.sub.2 COCH.sub.2 --, --COCH.sub.2 --, --C(.dbd.NOC(.dbd.O)NHQ)--, and --C(.dbd.NQ)NH--;

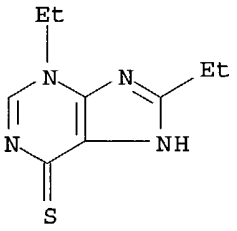
X.sub.1 and X.sub.2 may be the same or different and each is O or S;

wherein Q is R.sub.4 or hydrogen except that when Z.dbd.C(.dbd.NOCONHQ)--, R.sub.4 is not benzyl and R.sub.1 and R.sub.2 are both not hydrogen.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **162279-42-7P 162279-43-8P**
(preparation of purines, isoguanines, and dithioxanthines as phosphodiesterase-IV inhibitors)
RN 162279-42-7 USPATFULL
CN 6H-Purin-6-one, 3,8-diethyl-3,7-dihydro- (9CI) (CA INDEX NAME)



RN 162279-43-8 USPATFULL
CN 6H-Purine-6-thione, 3,8-diethyl-3,7-dihydro- (9CI) (CA INDEX NAME)



L6 ANSWER 18 OF 22 USPATFULL on STN

ACCESSION NUMBER:	1999:13044 USPATFULL
TITLE:	Methods for the synthesis of chemical compounds having PDE-IV inhibitory activity
INVENTOR(S):	Chasin, Mark, Manalapan, NJ, United States Cavalla, David, Cambridge, Great Britain Hofer, Peter, Liestal, Switzerland
PATENT ASSIGNEE(S):	Euro-Celtique, S.A., Luxembourg, Luxembourg (non-U.S. corporation)

	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 5864037		19990126	
APPLICATION INFO.:	US 1996-659767		19960606	(8)

DOCUMENT TYPE:	Utility
FILE SEGMENT:	Granted
PRIMARY EXAMINER:	Berch, Mark L.
LEGAL REPRESENTATIVE:	Davidson, Davidson & Kappel, LLC
NUMBER OF CLAIMS:	18
EXEMPLARY CLAIM:	1
LINE COUNT:	908

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Disclosed is a process for the preparation of a compound of Formula IV having the structure: ##STR1## wherein R.sub.6 is N(R.sub.6a)(R.sub.6b);

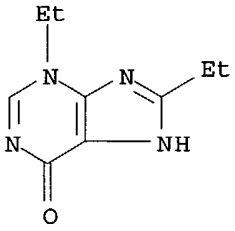
R.sub.3 represents a C.sub.2-8, alkyl which is unbranched or branched and unsubstituted or substituted; C.sub.3-8 cycloalkyl which is unsubstituted or substituted; C.sub.4-8 cycloalkylalkyl wherein the cycloalkyl portion is unsubstituted or substituted; aryl or benzyl which is optionally unsubstituted or substituted; ar(C.sub.1-4)alkyl; a heterocyclyl group, ring optionally substituted; heterocyclyl (C.sub.1 -C.sub.4) alkyl ring optionally substituted;

which comprises:

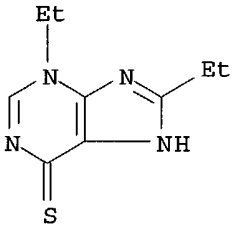
(a) treating a compound of Formula I: ##STR2## with an effective amount of a dethionating agent to produce a compound of Formula II: ##STR3## (b) treating a compound of Formula II with an effective halogenating agent under conditions effective to produce a compound of Formula III:

##STR4## and (c) treating a compound of Formula III with an effective aminating agent under conditions effective to produce a compound of Formula IV.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **162279-42-7P 162279-43-8P**
(preparation of purines, isoguanines, and dithioxanthines as phosphodiesterase-IV inhibitors)
RN 162279-42-7 USPATFULL
CN 6H-Purin-6-one, 3,8-diethyl-3,7-dihydro- (9CI) (CA INDEX NAME)



RN 162279-43-8 USPATFULL
CN 6H-Purine-6-thione, 3,8-diethyl-3,7-dihydro- (9CI) (CA INDEX NAME)

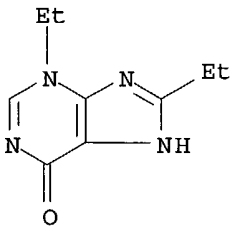


L6 ANSWER 19 OF 22 USPATFULL on STN
ACCESSION NUMBER: 97:81285 USPATFULL
TITLE: Substituted benzoxazoles
INVENTOR(S): Cavalla, John David, Cambridge, England
Dolby, Lloyd J., Eugene, OR, United States
Hofer, Peter, Liestal, Switzerland
Chasin, Mark, Manalapan, NJ, United States
PATENT ASSIGNEE(S): Euro-Celtique, S.A., Luxembourg, Luxembourg (non-U.S. corporation)

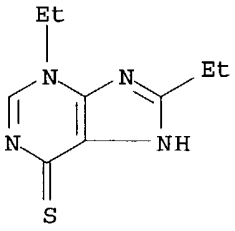
	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 5665737		19970909	
APPLICATION INFO.:	US 1994-321730		19941012	(8)

DOCUMENT TYPE: Utility
FILE SEGMENT: Granted
PRIMARY EXAMINER: Daus, Donald G.
LEGAL REPRESENTATIVE: Steinberg, Raskin & Davidson, P.C.
NUMBER OF CLAIMS: 24
EXEMPLARY CLAIM: 1
LINE COUNT: 986
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB Novel compounds which are effective PDE IV inhibitors are disclosed. The compounds possess improved PDE IV inhibition as compared to theophylline or rolipram, with improved selectivity with regard to, e.g., PDE III inhibition.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **162279-42-7P 162279-43-8P**
(preparation of purines, isoguanines, and dithioxanthines as phosphodiesterase-IV inhibitors)
RN 162279-42-7 USPATFULL
CN 6H-Purin-6-one, 3,8-diethyl-3,7-dihydro- (9CI) (CA INDEX NAME)



RN 162279-43-8 USPATFULL
CN 6H-Purine-6-thione, 3,8-diethyl-3,7-dihydro- (9CI) (CA INDEX NAME)



L6 ANSWER 20 OF 22 WPIDS COPYRIGHT 2004 THOMSON DERWENT on STN
**** DATA NOT AVAILABLE FOR THIS ACCESSION NUMBER

L6 ANSWER 21 OF 22 WPIDS COPYRIGHT 2004 THOMSON DERWENT on STN
**** DATA NOT AVAILABLE FOR THIS ACCESSION NUMBER

L6 ANSWER 22 OF 22 WPIDS COPYRIGHT 2004 THOMSON DERWENT on STN
**** DATA NOT AVAILABLE FOR THIS ACCESSION NUMBER

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	75.28	231.75

FILE 'REGISTRY' ENTERED AT 15:12:43 ON 25 MAY 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 24 MAY 2004 HIGHEST RN 685504-43-2
DICTIONARY FILE UPDATES: 24 MAY 2004 HIGHEST RN 685504-43-2

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

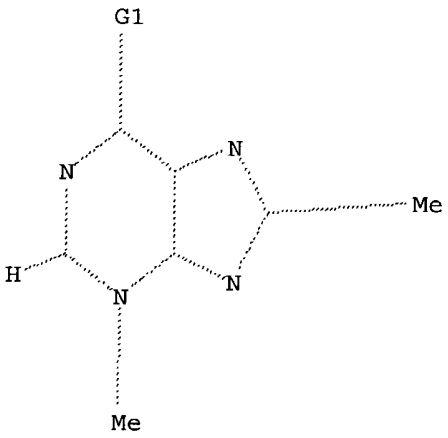
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\3,8-dimethyl- hypoxanthine.str

L7 STRUCTURE UPLOADED

=> d
L7 HAS NO ANSWERS
L7 STR



G1 O,S

Structure attributes must be viewed using STN Express query preparation.

=> s l7
SAMPLE SEARCH INITIATED 15:13:08 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 432 TO ITERATE

100.0% PROCESSED 432 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 7393 TO 9887
PROJECTED ANSWERS: 0 TO 0

L8 0 SEA SSS SAM L7

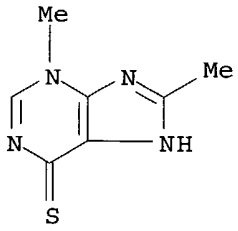
=> s l7 full
FULL SEARCH INITIATED 15:13:12 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 8709 TO ITERATE

100.0% PROCESSED 8709 ITERATIONS 15 ANSWERS
SEARCH TIME: 00.00.01

L9 15 SEA SSS FUL L7

=> d scan

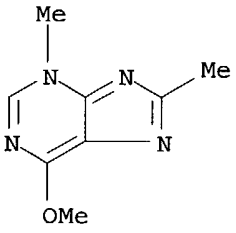
L9 15 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 6H-Purine-6-thione, 1,3-dihydro-3,8-dimethyl- (9CI)
MF C7 H8 N4 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

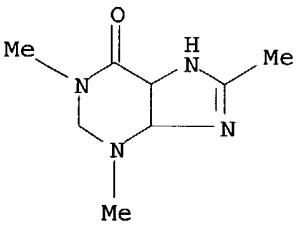
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):14

L9 15 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 3H-Purine, 6-methoxy-3,8-dimethyl- (9CI)
MF C8 H10 N4 O



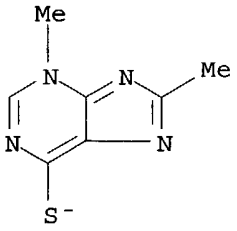
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 15 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 1H-Purinium, 4,5,6,7-tetrahydro-1,3,8-trimethyl-6-oxo-, iodide (9CI)
MF C8 H13 N4 O . I

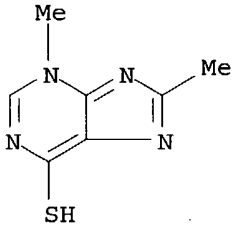


*** FRAGMENT DIAGRAM IS INCOMPLETE ***

L9 15 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 3H-Purine-6-thiol, 3,8-dimethyl-, ion(1-) (9CI)
MF C7 H7 N4 S

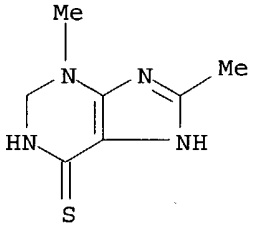


L9 15 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 3H-Purine-6-thiol, 3,8-dimethyl- (9CI)
MF C7 H8 N4 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

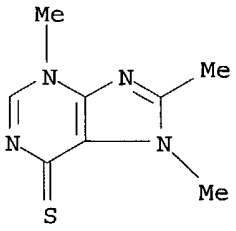
L9 15 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 6H-Purine-6-thione, 1,2,3,7-tetrahydro-3,8-dimethyl- (9CI)
MF C7 H10 N4 S



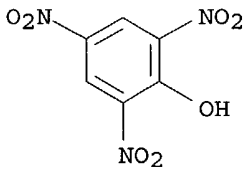
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 15 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Purine-6(3H)-thione, 3,7,8-trimethyl-, picrate (7CI, 8CI)
MF C8 H10 N4 S . C6 H3 N3 O7

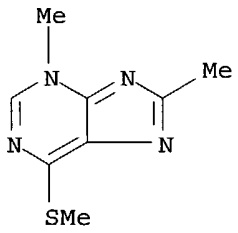
CM 1



CM 2

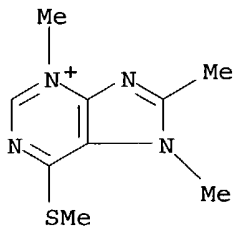


L9 15 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 3H-Purine, 3,8-dimethyl-6-(methylthio)- (7CI, 8CI, 9CI)
MF C8 H10 N4 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

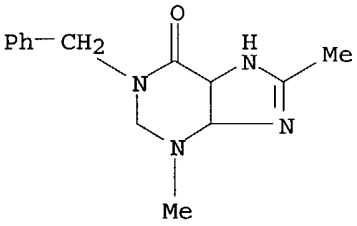
L9 15 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 3,7,8-Trimethyl-6-(methylthio)purinium iodide (7CI)
MF C9 H13 N4 S . I



● I^-

L9 15 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

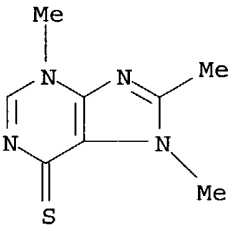
IN 1H-Purinium, 4,5,6,7-tetrahydro-3,8-dimethyl-6-oxo-1-(phenylmethyl)-, bromide (9CI)
MF C14 H17 N4 O . Br



● Br^-

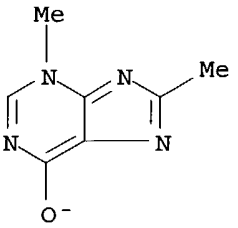
*** FRAGMENT DIAGRAM IS INCOMPLETE ***

L9 15 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 6H-Purine-6-thione, 3,7-dihydro-3,7,8-trimethyl- (9CI)
MF C8 H10 N4 S
CI COM



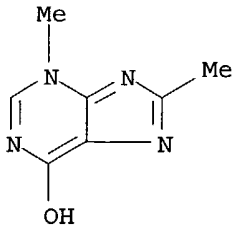
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 15 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 3H-Purin-6-ol, 3,8-dimethyl-, ion(1-) (9CI)
MF C7 H7 N4 O



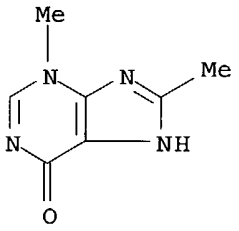
L9 15 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 3H-Purin-6-ol, 3,8-dimethyl- (9CI)

MF C7 H8 N4 O



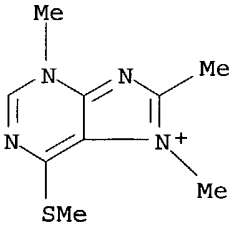
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 15 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 6H-Purin-6-one, 3,7-dihydro-3,8-dimethyl- (9CI)
MF C7 H8 N4 O



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 15 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Purinium, 3,7,8-trimethyl-6-(methylthio)-, iodide (8CI)
MF C9 H13 N4 S . I



ALL ANSWERS HAVE BEEN SCANNED

```
=> FIL MEDLIN HCAPL USPATF WPIDS
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   155.42     387.17

FILE 'MEDLINE' ENTERED AT 15:13:35 ON 25 MAY 2004

FILE 'HCAPLUS' ENTERED AT 15:13:35 ON 25 MAY 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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FILE 'USPATFULL' ENTERED AT 15:13:35 ON 25 MAY 2004
CA INDEXING COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'WPIDS' ENTERED AT 15:13:35 ON 25 MAY 2004
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=> s l9
SAMPLE SEARCH INITIATED 15:13:40 FILE 'WPIDS'
SAMPLE SCREEN SEARCH COMPLETED -     72 TO ITERATE

100.0% PROCESSED      72 ITERATIONS                          0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          466 TO      974
PROJECTED ANSWERS:               0 TO        0

L10         12 L9

=> dup rem l10
PROCESSING COMPLETED FOR L10
L11          12 DUP REM L10 (0 DUPLICATES REMOVED)

=> d ibib abs hitstr 10-12

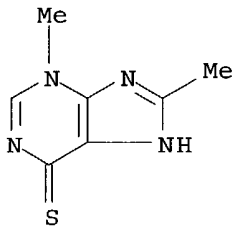
L11  ANSWER 10 OF 12  HCAPLUS  COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:         1966:104221  HCAPLUS
DOCUMENT NUMBER:          64:104221
ORIGINAL REFERENCE NO.:   64:19613b-d
TITLE:                    N-Alkylation of 6-methylthlopurines
AUTHOR(S):                Neiman, Z.; Bergmann, F.
CORPORATE SOURCE:         Handassah Med. School, Hebrew Univ., Jerusalem
SOURCE:                   Israel J. Chem. (1966), 3(5), 161-72
DOCUMENT TYPE:            Journal
LANGUAGE:                 English
AB   N-Methylation was carried out by refluxing 6-methylthiopurines with excess
     MeI in HCONMe2 (DMF) or MeCN, removing the solvent in vacuo, and crystallizing
     the residue.  The residue is purified as such or converted to the free
     base or corresponding betaine.  The compound prepared, the refluxing time
     (hrs.), the solvent used for methylation, and the m.p. of the product
     were: 3,7-dimethyl-6-methylthio purine iodide (yellow), 1.5, MeCN,
     193-4° (decomposition); 3,9-dimethyl-6-methylthlopurme iodide, 2, DMF,
     222° (decomposition); 1,9-dimethyl-6-methylthiopurine iodide, 3, DMF,
     217-19°; 2,3-dimethyl-6-methylthiopurine, 3, DMF, 192-4;
     3,7,8-trimethyl-6-methylthiopurine iodide, 2, MeCN, 213-14°.  For
     thiohydrolysis, 6-methylthio derivative was dissolved in 10% NH3, which had
     been saturated with H2S.  After bubbling H2S through the solution for an addnl.
     10 min., the 6-mercapto derivative was isolated directly or after evaporation
to
     dryness.  The yellow 6-mercaptopurines prepared were (substituent and m.p.
     given): 3,7-dimethyl, 282-3° (H2O); 3,9-dimethyl, 276-8°
```

(AcOH-benzene); 1,9-dimethyl, 250° (AcOH); 2,3-dimethyl, 295-7 (AcOH-benzene); 2,3,7-trimethyl, 298-9° (decomposition) (H2O-10% MeCN); 3,7,8-trimethyl, 175-8° (decomposition) (EtOH-MeCN). The mechanism of methylation is discussed.

IT **5098-06-6**, Purine-6(3H)-thione, 3,8-dimethyl- **5098-10-2**, 3H-Purine, 3,8-dimethyl-6-(methylthio)- **5759-69-3**, Purine-6(3H)-thione, 3,7,8-trimethyl-, picrate
(preparation of)

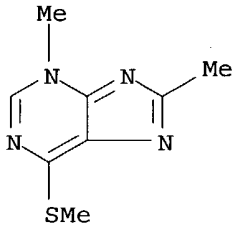
RN 5098-06-6 HCAPLUS

CN 6H-Purine-6-thione, 1,3-dihydro-3,8-dimethyl- (9CI) (CA INDEX NAME)



RN 5098-10-2 HCAPLUS

CN 3H-Purine, 3,8-dimethyl-6-(methylthio)- (7CI, 8CI, 9CI) (CA INDEX NAME)



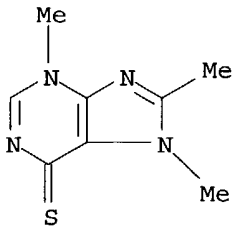
RN 5759-69-3 HCAPLUS

CN Purine-6(3H)-thione, 3,7,8-trimethyl-, picrate (7CI, 8CI) (CA INDEX NAME)

CM 1

CRN 46172-82-1

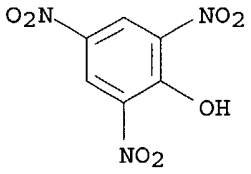
CMF C8 H10 N4 S



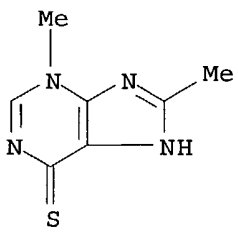
CM 2

CRN 88-89-1

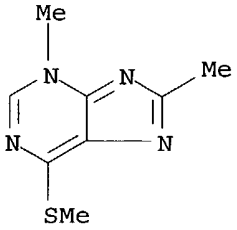
CMF C6 H3 N3 O7



L11 ANSWER 11 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1966:11492 HCAPLUS
DOCUMENT NUMBER: 64:11492
ORIGINAL REFERENCE NO.: 64:2087a-d
TITLE: Demethylation of 3-methyl-6-methylthiopurines with hydrogen sulfide
AUTHOR(S): Neiman, Z.; Bergmann, F.
CORPORATE SOURCE: Hebrew Univ.-Hadassah Med. School, Jerusalem
SOURCE: Israel J. Chem. (1965), 3(3), 85-9
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB The title compds., with the quinonoid form of the imidazole ring, readily undergo thiohydrolysis in aqueous solution (I, R = H), (II, R = H), (VII), , (VIII); (III, R = Me), (IV, R = Me), , , , , ; (V, R = Ph), (VI, R = Ph), , , , Thus, H2S bubbled during 20 min. at room temperature through a suspension of I in 25% NH4OH and the solution evaporated to dryness in vacuo gives 70% II. Similarly, III gives 60% IV, decomposed 300° (AcOH); V in Me2NCHO containing 0.1 volume N NaOH gives VI, decomposed 280-5° (dilute AcOH); and VII gives 80% VIII. 6-Methylthiopurine (non-quinonoid imidazole ring) is unchanged under the same conditions. A mixture of 22 g. 8-phenylhypoxanthine, 100 g. P2S5, and 500 ml. dry β-picoline was stirred and refluxed 4 hrs., the solvent removed in vacuo, the residue treated 1 hr. with 200 ml. H2O at 70°, the insoluble material triturated with 2N NaOH, and the mixture filtered through Celite. The solution was decolorized with C, acidified with AcOH, the precipitate dissolved in 5% Na2CO3, the solution heated with C, filtered, and cooled. The Na salt which separated was dissolved in hot H2O and hot saturated aqueous NH4Cl added to give 80% yellow needles of 6-mercapto-8-phenylpurine (IX), decomposed 300°. A solution of 39 g. IX in 600 ml. Me2NCHO containing 75 ml. MeI was refluxed 2 hrs., 40 ml. MeI added, reflux continued 2 hrs., and the mixture cooled. The yellow precipitate was dissolved in H2O and the pH adjusted to 10 with 2N NaOH to yield 48% V, m. 196-8° (iso-PrOH). Similarly, 6-mercapto-8-methylpurine gave 47% III, m. 195° (MeCN). A solution of 2.5 g. 6-thiotheophylline (VIII) in 15 ml. N NaOH stirred 4 hrs. at room temperature with 2.5 ml. MeI, neutralized with AcOH, evaporated to dryness in vacuo, and the residue extracted with iso-PrOH gave 22% VII, m. 189-91° (iso-PrOH). Uv and chromatographic data are given.
IT **5098-06-6**, Purine-6(3H)-thione, 3,8-dimethyl- **5098-10-2**, 3H-Purine, 3,8-dimethyl-6-(methylthio)-
(preparation of)
RN 5098-06-6 HCAPLUS
CN 6H-Purine-6-thione, 1,3-dihydro-3,8-dimethyl- (9CI) (CA INDEX NAME)



RN 5098-10-2 HCAPLUS
CN 3H-Purine, 3,8-dimethyl-6-(methylthio)- (7CI, 8CI, 9CI) (CA INDEX NAME)



L11 ANSWER 12 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1962:18329 HCAPLUS
DOCUMENT NUMBER: 56:18329
ORIGINAL REFERENCE NO.: 56:3480c-i,3481a-b
TITLE: Synthesis of 8-substituted purines
AUTHOR(S): Bergmann, F.; Tamari, M.
CORPORATE SOURCE: Hebrew Univ., Jerusalem, Israel
SOURCE: Journal of the Chemical Society, Abstracts (1961) 4468-72
CODEN: JCSAAZ; ISSN: 0590-9791
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 56:18329

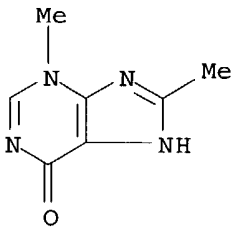
AB Condensation of an acetamidine salt with an appropriate derivative of 4,5-diaminopyrimidine in the absence of a solvent led directly to high yields of the 8-substituted purines (I). General procedure. A mixture of a 4,5diaminopyrimidine and 2 equivs. MeC(:NH)NH2.HCl (II.HCl) heated to 180-90° (homogeneous melt was formed and NH3 was evolved), when reaction ceased, the melt dissolved in N NaOH, the solution decolorized with C, and acidified with AcOH to pH 6 gave the I, all decomposing above 310° [substituents at 2-, 6-, and 8-position, reaction time in min., % yield, λ (mμ) at pH 8.0, Rf in 85:10:5 95% EtOH-H2OAcOH (solvent A), 70:20:10 95% EtOH-pyridine-H2O (solvent B), and 65:25:10 iso-PrOH-HCONMe2-10% aqueous NH3 (solvent C) given]: H, OH, Me, 60, 56 (the yield was improved by addition of 2 equivs. anhydrous NaOAc), 2.52, 0.57, 0.70, --; H, OH, Me, 60, 67 (with II.AcOH), --, --, --, --; OH, OH, Me, 30, 94, 240 and 275, 0.54, 0.60, 0.42; OH, SH, Me (III), 35, 83 (the yield was improved by addition of 2 equivs. anhydrous NaOAc) (the same compound was also prepared in 90% yield from 8-methylxanthine with P2S5), 251 and 344, 0.50, 0.56, 0.57; SH, OH, Me, 30, 77, 235 and 280, 0.45, 0.74, 0.61; SH, SH, Me, 25, 65 (the yield was improved with 2 equivs. anhydrous NaOAc), 247 and 285, and 351, 0.53, 0.59, 0.71; SH, SH, Me (IV), 25, 86 (with II.AcOH), --, --, --, --; SH, NH2, Me (V), 30, 66 (isolated as the sulfate), 230 and 251, and 280, 0.61, 0.67, --; H, OH, Ph, 70, 50, 291, 0.58, 0.79, --; H, OH, Ph, 70, 78 (with II.AcOH), --, --, --; OH, OH, Ph, 40, 80, 228 and 309, 0.52, 0.66, --. Also were prepared 92% 3,8-dimethylxanthine (VI), λ (pH 8.0) 275 m, Rf 0.64 (in A), 0.79 (in B), and 0.68 (in C), and 88% 3,8-dimethyl-2-mercaptoxanthine (VII), λ (pH 8.0), 233 and 288 mμ, Rf 0.60 (in A) and 0.84 (in B). N:C(OH).-N:C(NH2).C(NH2):CH (VIII) (Kalmus and Bergmann, CA 55, 12418h) (1 g.), 1 g. II.HCl, and 0.8 g. anhydrous NaOAc heated 20 min. at 140-5, the resulting cake dissolved in 10% aqueous NH3, the solution boiled with C, filtered, and the filtrate kept 24 hrs. in a cold room gave 0.65 g. inseparable mixture of VIII and 2-hydroxy-8-methylpurine (IX), (pH 8.0) 307 m. III (5 g.) and 1.5 g. (wet weight) Raney Ni in 25 ml. 5% aqueous NH3 refluxed 80 min., filtered, the filtrate adjusted to pH 2 with HNO3, and kept 2 months at room temperature gave IX.HNO3. If the above ammoniacal solution was acidified with H2SO4, IX

decomposed quant. The same result was obtained when an ammoniacal solution of IX was evaporated to dryness, the residue extracted with absolute EtOH, and the mixture acidified with 1% alc.-H_2SO_4. V (580 mg.) and 1.5 g. (wet weight) Raney Ni in 100 ml. 5% aqueous NH_2 refluxed 2 hrs., filtered hot, and the filtrate cooled gave 300 mg. 8-methyladenine, Rf 0.57 (in A), 0.67 (in B), and 0.64 (in C). 8-Methylhypoxanthine (1.3 g.), 5 g. P_2S_5, and 50 ml. dry pyridine refluxed 4 hrs., concentrated in vacuo, the residue extracted with 37 NaOH, filtered, the solution concentrated in vacuo, and kept overnight at 0° gave 1.1 g. 6-mercapto-8-methylpurine, decomposed above 310° (H_2O), (pH 8.0) 232 and 316 m, Rf 0.64 (in A) and 0.71 (in C). VII (1 g.) and 0.7 ml. MeI stirred 30 min. at room temperature in 10 ml. 0.5N NaOH gave 0.95 g. 3,8-dimethyl2-(methylthio)hypoxanthine, decomposed at 312-15° (H_2O), Rf 0.73 (in B). VII (2 g.) and 6 g. (wet weight) Raney Ni in 50 ml. 5% aqueous NH_3 refluxed 2 hrs., filtered, and concentrated in vacuo gave 1.4 g. 3,8-dimethylhypoxanthine, decomposed at 300° (EtOH), Rf 0.6 (in B). NH.CO.NMe.C(NH2):C- (NH2).CS (X) and II.HCl or II.AcOH heated at 150-200° gave only X and tars. VI treated with P_2S_5 in pyridine, concentrated in vacuo, the residue decomposed with cold dilute aqueous NH_3, the mixture filtered, and the filtrate adjusted to pH 6 with AcOH gave only X, λ (pH 8.0) 249 and 344 mμ, Rf 0.33 (in A). IV (1 g.) and 2.5 g. Raney Ni in 50 ml. 5% aqueous NH_3 refluxed 70 min., filtered, the filtrate concentrated in vacuo, and kept overnight gave 150 mg. 8-methylpurine, λ (pH 8.0) 266 mμ, Rf 0.75 (in A).

IT **25108-93-4**, Hypoxanthine, 3,8-dimethyl-
(preparation of)

RN 25108-93-4 HCAPLUS

CN 6H-Purin-6-one, 3,7-dihydro-3,8-dimethyl- (9CI) (CA INDEX NAME)



=> d ibib abs hitstr 1-9

L11 ANSWER 1 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1979:185947 HCAPLUS

DOCUMENT NUMBER: 90:185947

TITLE: Reactivities and electronic aspects of nucleic acid heterocycles. 8. Regioselective radical methylation of carbon-2 and carbon-8 of 6- and 3,6-substituted purines

AUTHOR(S): Zady, Mona F.; Wong, John L.

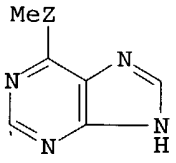
CORPORATE SOURCE: Dep. Chem., Univ. Louisville, Louisville, KY, USA

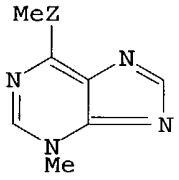
SOURCE: Journal of Organic Chemistry (1979), 44(9), 1450-4
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



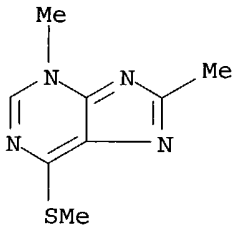
I


II

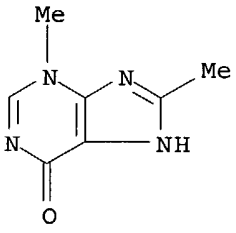
AB Pseudo 1st-order rate consts. were determined for methylation of hypoxanthine, its 3-Me derivative, and I (Z = O,S) and II (Z = O,S) in acidic and neutral media with Me• produced by the photolysis of AcOOCMe3. Under acid conditions, hypoxanthine and I yielded mainly 8-methylpurines. 3-Methylhypoxanthine and II were methylated mainly at the 2 position. This regioselectivity was correlated with the site of cation formation via 1H NMR anal. of the aromatic protons in acidic and neutral media. Methylation occurred fastest at the C atom whose proton resonated at lowest field in the acid NMR spectrum. In neutral solution, the regioselectivity was practically lost in the case of I and reversed to 8-methylation in the case of II. The results are compatible with an SEAr mechanism involving a radical σ complex.

IT **5098-10-2P 25108-93-4P 69257-63-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

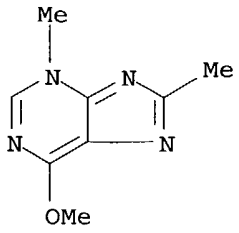
RN 5098-10-2 HCAPLUS
CN 3H-Purine, 3,8-dimethyl-6-(methylthio)- (7CI, 8CI, 9CI) (CA INDEX NAME)



RN 25108-93-4 HCAPLUS
CN 6H-Purin-6-one, 3,7-dihydro-3,8-dimethyl- (9CI) (CA INDEX NAME)



RN 69257-63-2 HCAPLUS
CN 3H-Purine, 6-methoxy-3,8-dimethyl- (9CI) (CA INDEX NAME)

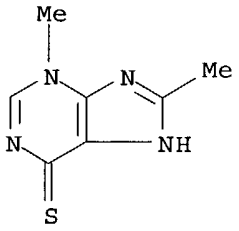


L11 ANSWER 2 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1977:67403 HCAPLUS
DOCUMENT NUMBER: 86:67403
TITLE: Influence of 8-substituents on the oxidation of hypoxanthine and 6-thioxopurine by bovine milk xanthine oxidase
AUTHOR(S): Bergmann, Felix; Levene, Lawrence; Govrin, Hanna; Frank, Aryeh
CORPORATE SOURCE: Hadassah Med. Sch., Hebrew Univ., Jerusalem, Israel
SOURCE: Biochimica et Biophysica Acta (1977), 480(1), 39-46
CODEN: BBACAQ; ISSN: 0006-3002
DOCUMENT TYPE: Journal
LANGUAGE: English

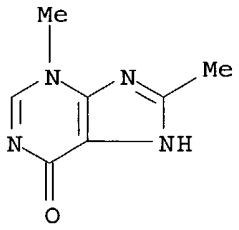
AB The effect of 8-substituents on the rate of oxidation of hypoxanthine and 6-thioxopurine by bovine milk xanthine oxidase was studied. An 8-Me group does not alter the rate of oxidation of hypoxanthine materially, but an 8-Ph substituent reduces it markedly. This is ascribed to inhibition of the tautomerization process, responsible for substrate activation, prior to oxidation In contrast, the 8-Ph group in 3-methyl-8-phenylhypoxanthine enhances the rate, presumably by binding to a hydrophobic site near the enzymic center. An 8-Ph group in 6-thioxopurine markedly increases the rate of enzymic oxidation Probably the aromatic substituent diverts anion formation to the imidazole ring. In contrast, ionization of 8-methyl-6-thioxopurine involves the pyrimidine moiety, thus rendering enzymic attack at position 2 more difficult.

IT **5098-06-6 25108-93-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxidation of, kinetics of enzymic)

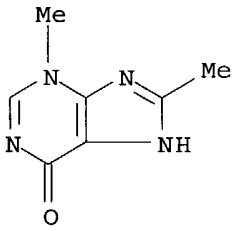
RN 5098-06-6 HCAPLUS
CN 6H-Purine-6-thione, 1,3-dihydro-3,8-dimethyl- (9CI) (CA INDEX NAME)



RN 25108-93-4 HCAPLUS
CN 6H-Purin-6-one, 3,7-dihydro-3,8-dimethyl- (9CI) (CA INDEX NAME)

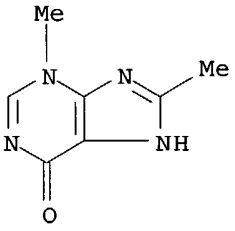


L11 ANSWER 3 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1976:416151 HCAPLUS
DOCUMENT NUMBER: 85:16151
TITLE: Oxidation of N-methyl substituted hypoxanthines, xanthines, purine-6,8-diones and the corresponding 6-thioxo derivatives by bovine milk xanthine oxidase
AUTHOR(S): Bergmann, Felix; Levene, Lawrence
CORPORATE SOURCE: Hadassah Med. Sch., Hebrew Univ., Jerusalem, Israel
SOURCE: Biochimica et Biophysica Acta (1976), 429(3), 672-88
CODEN: BBACAQ; ISSN: 0006-3002
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The oxidation of 6 series of purines (hypoxanthines, xanthines, purine-6,8-diones, and the corresponding 6-thioxo derivs.) by a highly purified bovine milk xanthine oxidase was studied, using a variety of N-Me derivs. N-Me substituents can either enhance or reduce enzymic rates. Enhancement is ascribed to blockage of groups which mediate unfavorable modes of binding of substrate to enzyme. Introduction of N-Me groups can also inhibit enzymic oxidation, either by occluding essential binding groups or by preventing spontaneous or enzyme-induced tautomerization processes, which create suitable binding sites in the substrates. In all purines which are rapidly attacked by xanthine oxidase, proper attachment to the active center is mediated by the groupings (3)NH, (9)N, or (3)N, (9)NH. Reduced rates usually express lowered substrate affinity, which finds its expression in weak competitive inhibition of xanthine oxidation
IT **25108-93-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxidation of, enzymic)
RN 25108-93-4 HCAPLUS
CN 6H-Purin-6-one, 3,7-dihydro-3,8-dimethyl- (9CI) (CA INDEX NAME)

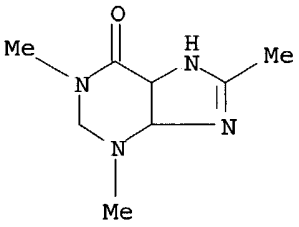


L11 ANSWER 4 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1976:105543 HCAPLUS
DOCUMENT NUMBER: 84:105543
TITLE: Thermal decomposition of quaternary hypoxanthinium salts and related purines
AUTHOR(S): Bergmann, Felix; Rahat, Miriam
CORPORATE SOURCE: Hadassah Med. Sch., Hebrew Univ., Jerusalem, Israel
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1976), (2), 239-43

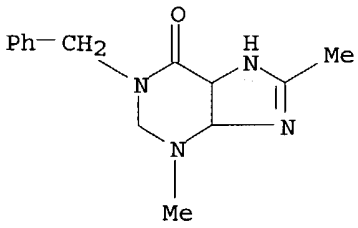
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Addnl. data considered in abstracting and indexing are available from a source cited in the original document. Thermal decomposition of quaternary hypoxanthinium salts was achieved by heating their solns. in DMF. 1,3-Dialkylhypoxanthinium bromides or iodides lost the 3-substituent as alkyl halide, which then attacked the imidazole ring at N-7 or N-9. Thermolysis of the dioxotetrahydropurinium iodide I (R = H) involved either loss of the 3-Me group as MeI giving the dihydromethylpurinedione II (R = H), or removal of HI to give the corresponding betaine which was then methylated at N-9 to give the dioxotetrahydropurinium iodide I (R = Me). The latter compound in turn decomposed to give the dimethylpurinedione II (R = Me). Similarly, the dimethylhypoxanthinium iodide III (R = H) was degraded mainly by loss of MeI, giving IV (R = H) and small amts. of V (R = H). III (R = H) also lost HI to give the corresponding betaine, which methylated at N-1 to give III (R = Me). III (R = Me) again underwent thermolysis to give a mixture of IV (R = Me) and its 9-Me isomer.
IT **25108-93-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with Me iodide)
RN 25108-93-4 HCAPLUS
CN 6H-Purin-6-one, 3,7-dihydro-3,8-dimethyl- (9CI) (CA INDEX NAME)



IT **59311-53-4 59311-56-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(thermal decomposition of)
RN 59311-53-4 HCAPLUS
CN 1H-Purinium, 4,5,6,7-tetrahydro-1,3,8-trimethyl-6-oxo-, iodide (9CI) (CA INDEX NAME)



*** FRAGMENT DIAGRAM IS INCOMPLETE ***
RN 59311-56-7 HCAPLUS
CN 1H-Purinium, 4,5,6,7-tetrahydro-3,8-dimethyl-6-oxo-1-(phenylmethyl)-, bromide (9CI) (CA INDEX NAME)



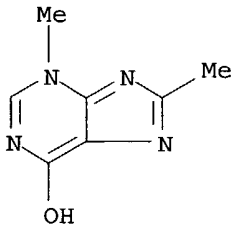
*** FRAGMENT DIAGRAM IS INCOMPLETE ***

L11 ANSWER 5 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1973:147123 HCAPLUS
DOCUMENT NUMBER: 78:147123
TITLE: Mechanism of hydrogen-deuterium exchange in hypoxanthines
AUTHOR(S): Lichtenberg, Dov; Bergmann, Felix
CORPORATE SOURCE: Dep. Pharmacol., Heb. Univ., Jerusalem, Israel
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1973), No. 8, 789-93
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English

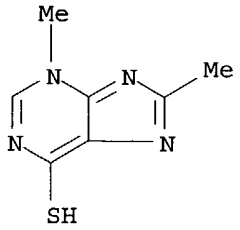
AB Kinetic studies on the H-D exchange reactions of 1-, 7-, and 9-methylhypoxanthine and 1,6-, 1,9-, and 7,9-dimethylhypoxanthine showed that the first aromatic proton to undergo exchange was that at C-8. 3-Methyl- and 3,7-dimethylhypoxanthine underwent exchange at C-2 first. Except for 1-methylhypoxanthine the corresponding anions react faster. The exchange proceeded by a protonation-deprotonation mechanism, which for anions involved formation of a zwitterion as the reactive species. Where zwitterion formation was impossible, as in the dianion of hypoxanthine or the monoanion of its 1-Me derivative, the exchange was very slow.

IT **41491-73-0 41491-74-1 41491-76-3**
41491-77-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(exchange reaction of, mechanism and kinetics of)

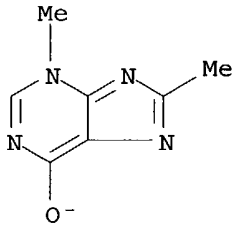
RN 41491-73-0 HCAPLUS
CN 3H-Purin-6-ol, 3,8-dimethyl- (9CI) (CA INDEX NAME)



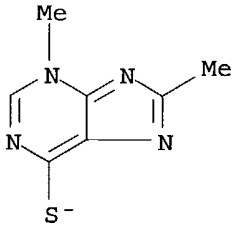
RN 41491-74-1 HCAPLUS
CN 3H-Purine-6-thiol, 3,8-dimethyl- (9CI) (CA INDEX NAME)



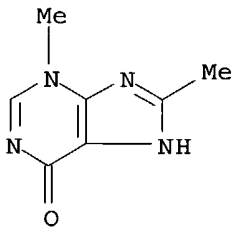
RN 41491-76-3 HCAPLUS
CN 3H-Purin-6-ol, 3,8-dimethyl-, ion(1-) (9CI) (CA INDEX NAME)



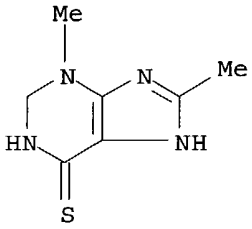
RN 41491-77-4 HCAPLUS
CN 3H-Purine-6-thiol, 3,8-dimethyl-, ion(1-) (9CI) (CA INDEX NAME)



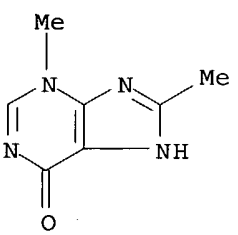
L11 ANSWER 6 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1972:474416 HCAPLUS
DOCUMENT NUMBER: 77:74416
TITLE: Assignment of individual signals of aromatic protons in the NMR spectrum of 6-substituted purines
AUTHOR(S): Lichtenberg, D.; Bergmann, F.; Ringel, I.
CORPORATE SOURCE: Hadassah Med. Sch., Hebrew Univ., Jerusalem, Israel
SOURCE: Journal of Magnetic Resonance (1969-1992) (1972), 6(4), 600-4
CODEN: JOMRA4; ISSN: 0022-2364
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Assignment of the resonances of ring protons in substituted purines is made by comparison with the NMR of compds. in which 1 of these protons is substituted by an alkyl group, and by application of the nuclear Overhauser effect to these derivs. in order to identify the signals of protons adjacent to the alkyl substituent. Chemical shifts are given for various ionic forms of the purines in D2O, as well as for the neutral forms.
IT **25108-93-4 38917-32-7**
RL: PRP (Properties)
(NMR of)
RN 25108-93-4 HCAPLUS
CN 6H-Purin-6-one, 3,7-dihydro-3,8-dimethyl- (9CI) (CA INDEX NAME)



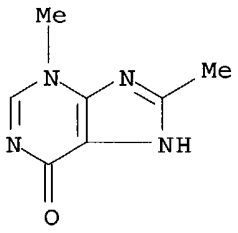
RN 38917-32-7 HCAPLUS
CN 6H-Purine-6-thione, 1,2,3,7-tetrahydro-3,8-dimethyl- (9CI) (CA INDEX NAME)



L11 ANSWER 7 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1971:505114 HCAPLUS
DOCUMENT NUMBER: 75:105114
TITLE: NMR spectra and ionization processes of hypoxanthines
AUTHOR(S): Bergmann, F.; Lichtenberg, D.; Neiman, Z.
CORPORATE SOURCE: Hadassah Med. Sch., Hebrew Univ., Jerusalem, Israel
SOURCE: Quantum Aspects Heterocycl. Compounds Chem. Biochem., Proc. Int. Symp., 2nd (1970), Meeting Date 1969, 314-23. Editor(s): Bergmann, Ernst D. Israel Acad. Sci. Hum.: Jerusalem, Israel.
CODEN: 23ULAG
DOCUMENT TYPE: Conference
LANGUAGE: English
AB The NMR spectra of hypoxanthine and its Me derivative were studied as a 1st approach to solution of the general problem of localization of ionized groups. It was concluded that only a charge in the immediate vicinity of the CH group at positions 2 or 8 influences the chemical shift of its H. Thus, a charge at position 7 or 9 would mainly influence the signal of the H atom on C-8, while ionization processes at one of the N atoms in the pyrimidine ring would mainly shift the band of the H atom on C-2.
IT **25108-93-4**
RL: PROC (Process)
(ionization of, N.M.R. in relation to)
RN 25108-93-4 HCAPLUS
CN 6H-Purin-6-one, 3,7-dihydro-3,8-dimethyl- (9CI) (CA INDEX NAME)



L11 ANSWER 8 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1969:512270 HCAPLUS
DOCUMENT NUMBER: 71:112270
TITLE: Hydrogen-deuterium exchange in hypoxanthines
AUTHOR(S): Bergmann, Felix; Lichtenberg, D.; Neiman, Z.
CORPORATE SOURCE: Hadassah Med. Sch., Hebrew Univ., Jerusalem, Israel
SOURCE: Journal of the Chemical Society [Section] D: Chemical Communications (1969), (17), 992-3
CODEN: CCJDAO; ISSN: 0577-6171
DOCUMENT TYPE: Journal
LANGUAGE: English
AB N.M.R. showed H-D exchange in D2O at 70-85° occurred at position 8 of hypoxanthine and of 7-methyl-, 2-chloro-7-methyl-, and 9-methylhypoxanthine, and at position 2 of 1,8-dimethyl-, 3-methyl-, 3,8-dimethyl-, and 7-methylhypoxanthine. The deuteration was fast at alkaline pH, slow at neutral pH and nil at pH 0. The activation energy for the exchange of 3-methylhypoxanthine was independent of the pH, suggesting the same deuteration mechanism for the neutral and the neg. charged forms.
IT **25108-93-4**
RL: PRP (Properties)
(exchange of hydrogen with deuterium in)
RN 25108-93-4 HCAPLUS
CN 6H-Purin-6-one, 3,7-dihydro-3,8-dimethyl- (9CI) (CA INDEX NAME)



L11 ANSWER 9 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1968:69047 HCAPLUS
DOCUMENT NUMBER: 68:69047
TITLE: Preparing 3-methyl-6-thionopurines from 3-methyl-6-methylthiopurines
INVENTOR(S): Bergmann, Felix; Neiman, Zohar; Rashi, Moshe
PATENT ASSIGNEE(S): Yissum Research Development Co.
SOURCE: Brit., 8 pp.
CODEN: BRXXAA
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

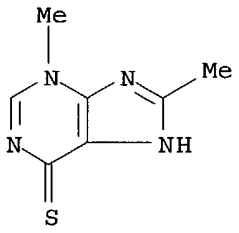
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 1073039		19670621		
IL 24642			IL	

PRIORITY APPLN. INFO.: IL 19651118
GI For diagram(s), see printed CA Issue.
AB The title reaction is effected with H2S in concentrated aqueous NH3. Thus, a mixture of 22 g. 8-methyl-6-thionopurine, 250 ml. dry HCONMe2 and 30 ml. MeI is refluxed 2 hrs., 15 ml. MeI added, the mixture again refluxed 2 hrs. to give 12 g. Ia (R1 = H, R2 = Me) (I). I (2 g.) is suspended in 50 ml. 25% aqueous NH3 and H2S bubbled through at room temperature for 20 min. to give 1.1 g. Ib (R1 = R2 = H, R3 = Me) decompose 300° (HOAc). Similarly prepared are

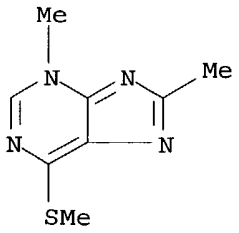
Ia (R1 = H, R2 = Ph), m. 196-8° (iso-PrOH) and Ib (R1 = R2 = H, R3 = Ph), decompose 280-5° (dilute HOAc). A solution of 2.5 g. 6-thiotheophylline in 15 ml. N, NaOH is stirred 4 hrs. with 2.5 ml. MeI at room temperature to give 0.6 g. 1,3-dimethyl-6-methylthio-2-oxopurine, m. 189-91° (MeCN), iso-PrOH), which can be converted with H2S/NH3 to 6-thionotheophylline in 80% yield. A solution of 4 g. Ia (R1 = R2 = H) (II) in 80 ml. MeCN is refluxed with 20 ml. MeI for 90 min. to give II.MeI (III), decompose 195-7°; 2 g. III is dissolved in 30 ml. concentrated aqueous NH3 which had been saturated with H2S, H2S bubbled through at room temperature for 10 min. after which Ib (R1 = R3 = H, R2 = Me), decompose 282-3° (H2O) forms. Also prepared is Ib (R1 = H, R2 = Me, R3 = Ph, m. 242° (HOAc), 4-amino-5-benzamido-6-methylthiopyrimidine, decompose .apprx. 250°; its N-Me analog, m. 214°; 7-methyl-6-methylthio-8-phenylpurine, m. 177°; Ia (R1 = Me, R2 = H), m. 192-4°; Ic (R1 = Me, R2 = R3 = H) decompose 295-7°; Ib (R1 = R2 = Me, R3 = H), decompose 298-9°; 8-(2-pyridyl)hypoxanthine, decompose >300°; 6-thiono-8-(2-pyridyl)purine, decompose >300° (HOAc); Ia (R1 = H, R2 = 2-pyridyl), m. 252°; Ib (R1 = R2 = H, R3 = 2-pyridyl), m. 266°. Details are also provided, for the intermediates and end-products, of λmaximum, log εmaximum, Rf and color of fluorescence.

IT **5098-06-6P 5098-10-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 5098-06-6 HCAPLUS
CN 6H-Purine-6-thione, 1,3-dihydro-3,8-dimethyl- (9CI) (CA INDEX NAME)



RN 5098-10-2 HCAPLUS
CN 3H-Purine, 3,8-dimethyl-6-(methylthio)- (7CI, 8CI, 9CI) (CA INDEX NAME)



=> FIL STNGUIDE

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	72.63	459.80

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-8.32	-8.32

FILE 'STNGUIDE' ENTERED AT 15:17:39 ON 25 MAY 2004
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AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: May 21, 2004 (20040521/UP).

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.48	460.28

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-8.32

FILE 'REGISTRY' ENTERED AT 15:22:22 ON 25 MAY 2004
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STRUCTURE FILE UPDATES: 24 MAY 2004 HIGHEST RN 685504-43-2
DICTIONARY FILE UPDATES: 24 MAY 2004 HIGHEST RN 685504-43-2

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=> fil marpat

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.42	460.70

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-8.32

FILE 'MARPAT' ENTERED AT 15:22:28 ON 25 MAY 2004
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FILE CONTENT: 1988-PRESENT (VOL 140 ISS 21)(20040521/ED)

MOST RECENT CITATIONS FOR PATENTS FROM FIVE MAJOR ISSUING AGENCIES
(COVERAGE TO THESE DATES IS NOT COMPLETE):

US 6727389 27 APR 2004
DE 10351214 08 APR 2004
EP 1406339 07 APR 2004
JP 2004123716 22 APR 2004
WO 2004035062 29 APR 2004

```
Structure search limits have been raised.  See HELP SLIMIT for the new,
higher limits.

=> s l7
SAMPLE SEARCH INITIATED 15:22:54 FILE 'MARPAT'
SAMPLE SCREEN SEARCH COMPLETED -     160 TO ITERATE

100.0% PROCESSED     160 ITERATIONS                              1 ANSWERS
SEARCH TIME: 00.00.02

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          2445 TO     3955
PROJECTED ANSWERS:                1 TO       80

L12           1 SEA SSS SAM L7

=> d

L12  ANSWER 1 OF 1  MARPAT  COPYRIGHT 2004 ACS on STN
AN   130:237812  MARPAT
TI   Preparation and use of pentopyranosyl-nucleosides
IN   Miculka, Christian; Windhab, Norbert; Brandstetter, Tilmann; Burdinski,
     Gerhard
PA   Hoechst A.-G., Germany
SO   Ger. Offen., 40 pp.
     CODEN: GWXXBX
DT   Patent
LA   German
FAN.CNT 1
     PATENT NO.        KIND  DATE           APPLICATION NO.  DATE
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     WO 9915539         A3   19990617
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         RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
             PT, SE
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         W:  AU, BR, CA, JP, KR, US
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     AU 9910245         A1   19990412       AU 1999-10245    19980921
     AU 757983          B2   20030313
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     EP 1017703         B1   20040428
         R:  AT, CH, DE, FR, GB, IT, LI, NL
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     EP 1017704         B1   20040225
         R:  AT, CH, DE, FR, GB, IT, LI, NL
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     JP 2001517675      T2   20011009       JP 2000-512845   19980921
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     BR 9812381         A    20020430       BR 1998-12381    19980921
     AT 233272          E    20030315       AT 1998-950062   19980921
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     US 6506896         B1   20030114       US 2000-509039   20000711
     US 6608186         B1   20030819       US 2000-509058   20000727
     US 2003039997      A1   20030227       US 2002-150402   20020516
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     WO 1998-EP5998    19980921
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=> s l7 exa
'EXA' IS NOT A VALID SEARCH TYPE
For an explanation, enter "HELP SEARCH TYPES"

=> fil reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                      ENTRY    SESSION
FULL ESTIMATED COST                                    3.11     463.81

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                      ENTRY    SESSION
CA SUBSCRIBER PRICE                                    0.00      -8.32

FILE 'REGISTRY' ENTERED AT 15:25:23 ON 25 MAY 2004
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provided by InfoChem.

STRUCTURE FILE UPDATES:   24 MAY 2004  HIGHEST RN 685504-43-2
DICTIONARY FILE UPDATES:  24 MAY 2004  HIGHEST RN 685504-43-2

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\hypoxanthine c.str

L13     STRUCTURE UPLOADED

=> d
L13 HAS NO ANSWERS
L13             STR
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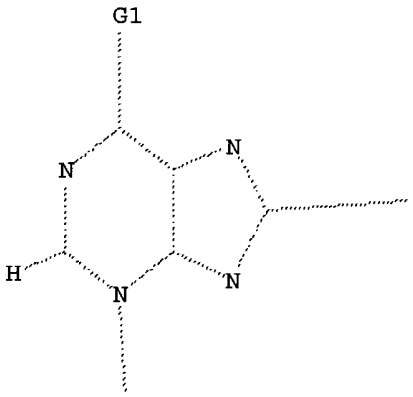

G1 O,S

Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SCREEN SEARCH COMPLETED -    432 TO ITERATE

100.0% PROCESSED     432 ITERATIONS                              1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          7393 TO     9887
PROJECTED ANSWERS:                1 TO       80

L14            1 SEA SSS SAM L13

=> d

L14  ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2004 ACS on STN
RN   162279-42-7  REGISTRY
CN   6H-Purin-6-one, 3,8-diethyl-3,7-dihydro- (9CI)  (CA INDEX NAME)
OTHER NAMES:
CN   3,8-Diethylhypoxanthine
FS   3D CONCORD
MF   C9 H12 N4 O
SR   CA
LC   STN Files:   CA, CAPLUS, USPATFULL
DT.CA  CAplus document type:  Patent
RL.P   Roles from patents:  BIOL (Biological study); PREP (Preparation); RACT
       (Reactant or reagent); USES (Uses)
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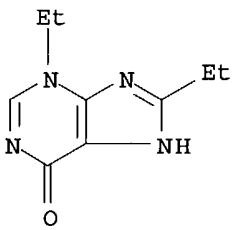

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**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

               4 REFERENCES IN FILE CA (1907 TO DATE)
               4 REFERENCES IN FILE CAPLUS (1907 TO DATE)


=> s l13 full
FULL SEARCH INITIATED 15:26:06 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   8709 TO ITERATE

100.0% PROCESSED    8709 ITERATIONS                                39 ANSWERS
SEARCH TIME: 00.00.01

L15          39 SEA SSS FUL L13

=> d his

     (FILE 'HOME' ENTERED AT 15:01:15 ON 25 MAY 2004)

     FILE 'REGISTRY' ENTERED AT 15:01:47 ON 25 MAY 2004
L1              STRUCTURE UPLOADED
L2            0 S L1
L3           39 S L1 FULL

     FILE 'MEDLINE, HCAPLUS, USPATFULL, WPIDS' ENTERED AT 15:03:50 ON 25 MAY
     2004
L4           47 S L3
L5           46 DUP REM L4 (1 DUPLICATE REMOVED)
L6           22 S L5 NOT PY>1999

     FILE 'REGISTRY' ENTERED AT 15:12:43 ON 25 MAY 2004
L7              STRUCTURE UPLOADED
L8            0 S L7
L9           15 S L7 FULL

     FILE 'MEDLINE, HCAPLUS, USPATFULL, WPIDS' ENTERED AT 15:13:35 ON 25 MAY
     2004
L10          12 S L9
L11          12 DUP REM L10 (0 DUPLICATES REMOVED)

     FILE 'STNGUIDE' ENTERED AT 15:17:39 ON 25 MAY 2004

     FILE 'REGISTRY' ENTERED AT 15:22:22 ON 25 MAY 2004

     FILE 'MARPAT' ENTERED AT 15:22:28 ON 25 MAY 2004
L12           1 S L7

     FILE 'REGISTRY' ENTERED AT 15:25:23 ON 25 MAY 2004
L13             STRUCTURE UPLOADED
L14           1 S L13
L15          39 S L13 FULL

=> s l15 not l13
L15 MAY NOT BE USED HERE
The L-number entered was not created by a STRUCTURE or SCREEN command.

=> s l15 not l3
L16          0 L15 NOT L3

=> fil stng
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                             157.61     621.42
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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-8.32

FILE 'STNGUIDE' ENTERED AT 15:26:43 ON 25 MAY 2004

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: May 21, 2004 (20040521/UP).

=>

---Logging off of STN---

Connection closed by remote host
END

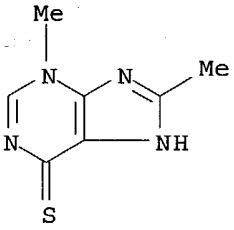
Unable to generate the STN prompt.
Exiting the script...

ACCESSION NUMBER: 1977:67403 HCAPLUS
DOCUMENT NUMBER: 86:67403
TITLE: Influence of 8-substituents on the oxidation of hypoxanthine and 6-thioxopurine by bovine milk xanthine oxidase
AUTHOR(S): Bergmann, Felix; Levene, Lawrence; Govrin, Hanna; Frank, Aryeh
CORPORATE SOURCE: Hadassah Med. Sch., Hebrew Univ., Jerusalem, Israel
SOURCE: Biochimica et Biophysica Acta (1977), 480(1), 39-46
CODEN: BBACAQ; ISSN: 0006-3002
DOCUMENT TYPE: Journal
LANGUAGE: English

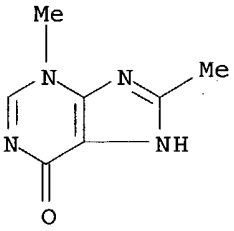
AB The effect of 8-substituents on the rate of oxidation of hypoxanthine and 6-thioxopurine by bovine milk xanthine oxidase was studied. An 8-Me group does not alter the rate of oxidation of hypoxanthine materially, but an 8-Ph substituent reduces it markedly. This is ascribed to inhibition of the tautomerization process, responsible for substrate activation, prior to oxidation In contrast, the 8-Ph group in 3-methyl-8-phenylhypoxanthine enhances the rate, presumably by binding to a hydrophobic site near the enzymic center. An 8-Ph group in 6-thioxopurine markedly increases the rate of enzymic oxidation Probably the aromatic substituent diverts anion formation to the imidazole ring. In contrast, ionization of 8-methyl-6-thioxopurine involves the pyrimidine moiety, thus rendering enzymic attack at position 2 more difficult.

IT **5098-06-6 25108-93-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxidation of, kinetics of enzymic)

RN 5098-06-6 HCAPLUS
CN 6H-Purine-6-thione, 1,3-dihydro-3,8-dimethyl- (9CI) (CA INDEX NAME)



RN 25108-93-4 HCAPLUS
CN 6H-Purin-6-one, 3,7-dihydro-3,8-dimethyl- (9CI) (CA INDEX NAME)



L11 ANSWER 3 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1976:416151 HCAPLUS
DOCUMENT NUMBER: 85:16151
TITLE: Oxidation of N-methyl substituted hypoxanthines, xanthines, purine-6,8-diones and the corresponding 6-thioxo derivatives by bovine milk xanthine oxidase
AUTHOR(S): Bergmann, Felix; Levene, Lawrence
CORPORATE SOURCE: Hadassah Med. Sch., Hebrew Univ., Jerusalem, Israel

SOURCE: Biochimica et Biophysica Acta (1976), 429(3), 672-88
CODEN: BBACAQ; ISSN: 0006-3002
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The oxidation of 6 series of purines (hypoxanthines, xanthines, purine-6,8-diones, and the corresponding 6-thioxo derivs.) by a highly purified bovine milk xanthine oxidase was studied, using a variety of N-Me derivs. N-Me substituents can either enhance or reduce enzymic rates. Enhancement is ascribed to blockage of groups which mediate unfavorable modes of binding of substrate to enzyme. Introduction of N-Me groups can also inhibit enzymic oxidation, either by occluding essential binding groups or by preventing spontaneous or enzyme-induced tautomerization processes, which create suitable binding sites in the substrates. In all purines which are rapidly attacked by xanthine oxidase, proper attachment to the active center is mediated by the groupings (3)NH, (9)N, or (3)N, (9)NH. Reduced rates usually express lowered substrate affinity, which finds its expression in weak competitive inhibition of xanthine oxidation

IT **25108-93-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxidation of, enzymic)

RN 25108-93-4 HCAPLUS

CN 6H-Purin-6-one, 3,7-dihydro-3,8-dimethyl- (9CI) (CA INDEX NAME)